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Luttinger parameters of interacting fermions in one dimension at high energies

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Interactions between electrons in one dimension are fully described at low energies by only a few parameters of the Tomonaga-Luttinger model, which is based on linearization of the spectrum. We consider a model of spinless fermions with short-range interaction via the Bethe-Ansatz technique and show that a Luttinger parameter emerges in an observable beyond the low-energy limit. A distinct feature of the spectral function, the edge that marks the lowest possible excitation energy for a given momentum, is parabolic for arbitrary momenta and the prefactor is a function of the Luttinger parameter, K .

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I. INTRODUCTION

The effects of interactions between fermions in one dimension are mainly understood at low energies within the scope of the Tomonaga-Luttinger model.¹ This framework is based on the linear approximation to the single-particle spectrum around the Fermi energy and provides, via the bosonization technique,¹ a generic way to calculate various correlation functions. Understanding of interacting fermions beyond the low-energy limit still presents a challenge. Studies are currently focused on dynamical response functions,²⁻⁷ e.g., the spectral function which can be measured by momentum-resolved tunneling of electrons in semiconductors,^{8,9} by angle-resolved photoemission in correlated materials¹⁰ and by photoemission spectroscopy in cold atoms.¹¹ Recently significant theoretical progress was achieved in this direction by making a connection between Luttinger liquids and the Fermi edge singularity problem.¹² As a result, power-law singularities were found at the edge of the spectral function at zero temperature and their powers were related to the corresponding curvature.¹³ The edge marks the smallest energy at a fixed momentum with which a particle can tunnel into the system. At low energies the edge disperses linearly with a slope which is the sound velocity of collective modes v defined by parameters from the Tomonaga-Luttinger model;¹⁴ a small quadratic correction to the linear slope at low momenta was found in Ref. 3. In this paper we calculate the position of the edge for the spinless fermions with a short-range interaction at arbitrary energies and show that a Luttinger parameter is still relevant at large energies.

Our strategy is to consider the exact diagonalization of the model on a lattice via the Bethe-Ansatz approach. Then we analyze the spectral function in the continuum regime—a combination of the thermodynamic limit and a small occupancy of the lattice¹⁵—which corresponds to the continuum model with a contact interaction. In this regime we find that the position of the edge is parabolic for arbitrary momenta and the prefactor is a function of the dimensionless Luttinger parameter K [see Eq. (10)], which is defined in the low-energy domain of the Tomonaga-Luttinger model. Our result could be directly observed in experiments on spin-polarized particles such as electrons in ferromagnetic semiconductors¹⁶ using the setups of Refs. 8 and 9 or polarized cold atoms using the setup of Ref. 11. In closely related models of spin chains,¹ the position of the edge depends on the Luttinger K in an analogous way, but for a

weakly polarized chain, for example, the parabolic function of momentum becomes a cosine. With the parabolic shape found in this paper, the phenomenological nonlinear Luttinger liquid theory¹³ gives a divergent power of the edge singularity.

In the continuum regime the Luttinger parameter K is bounded and the smallest K for large interaction strengths is almost degenerate with its noninteracting value $K = 1$. We use the Bethe-Ansatz approach for a finite-range interaction potential beyond nearest neighbor in the limit $V = \infty$ and show that the regime of strong interaction effects (corresponding to the minimum value of $K = 0$ in the Tomonaga-Luttinger model) can only be accessed by a microscopic model with the interaction range at least of the order of the average distance between particles.

The paper is organized as follows. Section II contains a definition of the model of spinless fermions on a lattice and the spectral function. In Sec. III we analyze the edge of the spectral function for next-neighbor interaction in the low (Sec. A) and high (Sec. B) regimes. In Sec. IV we consider a finite-range interaction in the limit of infinite interaction strength. In the Appendix we give numerical data that clarify the calculations in Secs. III and IV.

II. MODEL

Spinless fermions on a one-dimensional lattice with L sites interact via a two-body potential V_i as

$$H = -t \sum_{j=1}^L (c_j^\dagger c_{j+1} + c_j^\dagger c_{j-1}) + \sum_{j=1, i=1}^{L, \infty} V_i c_j^\dagger c_j c_{j+i}^\dagger c_{j+i}, \quad (1)$$

where t is a hopping amplitude and operators c_j obey Fermi commutation relations $\{c_i, c_j^\dagger\} = \delta_{ij}$.¹⁷ Below we consider periodic boundary conditions $c_{L+1} = c_1$ to maintain the translation symmetry of the finite length chain and consider only repulsive interactions, $V_i > 0$.

The spectral function describes the tunneling probability for a particle with momentum k and energy ε , $A(k, \varepsilon) = -\text{Im}G(k, \varepsilon) \text{sgn}(\varepsilon - \mu)/\pi$, where μ is the chemical potential and $G(k, \varepsilon) = -i \sum_j \int dt e^{i(kj - \varepsilon t)} \langle T(e^{-iHt} c_j e^{iHt} c_1^\dagger) \rangle / L$ is a Fourier transform of the single-particle Green function at zero temperature. To be specific, we discuss only a particular region, $k_F < k < 3k_F$ and $\varepsilon > \mu$. The spectral function in this domain

reads¹⁸

$$A(k, \varepsilon) = L \sum_f |\langle f | c_1^\dagger | 0 \rangle|^2 \delta(k - P_f) \delta(\varepsilon + E_0 - E_f), \quad (2)$$

where E_0 is the energy of the ground state $|0\rangle$, and P_f and E_f are the momenta and the eigenenergies of the eigenstates $|f\rangle$; all eigenstates are assumed normalized.

III. NEXT-NEIGHBOR INTERACTION

The model of Eq. (1) can be diagonalized using the Bethe Ansatz when the interaction potential is restricted to the nearest neighbor only, $V_i = V\delta_{i,1}$.¹⁹ In the coordinate basis, $|\psi\rangle = \sum_{j_1 < \dots < j_n} a_{j_1 \dots j_n} c_{j_1}^\dagger \dots c_{j_n}^\dagger |\text{vac}\rangle$, where $|\text{vac}\rangle$ is the fermionic vacuum, a superposition of plain waves, $a_{j_1 \dots j_n} = \sum_P e^{i \sum_{i=1}^n k_{P_i} j_i + i \sum_{i < m=1}^n \varphi_{P_i, P_m}}$, is an n particle eigenstate and $H|\psi\rangle = E|\psi\rangle$ with the eigenenergy

$$E = -2t \sum_{j=1}^n \cos(k_j) + 2tn. \quad (3)$$

Here a constant $2tn$ was added for convenience, the phase shifts

$$e^{i2\varphi_{jm}} = - \frac{e^{i(k_j+k_m)} + 1 + \frac{V}{t} e^{ik_j}}{e^{i(k_j+k_m)} + 1 + \frac{V}{t} e^{ik_m}} \quad (4)$$

are fixed by the two-body scattering problem, and \sum_P is a sum over all permutations of n integer numbers. The periodic boundary condition quantizes all single-particle momenta simultaneously,

$$Lk_j - 2 \sum_m \varphi_{jm} = 2\pi\lambda_j, \quad (5)$$

where λ_j are integer numbers. The sum $P = \sum_j k_j$ is a conserved quantity—the total momentum of an n particle state.

The solutions of the nonlinear system of equations Eq. (5) can be classified in the limit of noninteracting particles. Under substitution of the scattering phase $2\varphi_{jm} = \pi$ for $V = 0$, Eq. (5) decouples into a set of independent quantization conditions for plain waves,

$$k_j = \frac{2\pi\lambda_j}{L}. \quad (6)$$

The corresponding eigenstates are Slater determinants which vanish when the momenta of any two particles are equal. Thus all eigenstates are mapped onto all possible sets of n nonequal integer numbers λ_j with $-L/2 < \lambda_j \leq L/2$. In the absence of bound-state formation, these solutions are adiabatically continued under a smooth deformation from $V = 0$ to any finite value of V . This permits us to use the free-particle classification to label many-particle states for an arbitrary interaction strength.

The limit of infinitely strong repulsion corresponds to free fermions of a finite size. The scattering phase $\varphi_{jm} = k_j - k_m + \pi$ for $V = \infty$ makes Eq. (5) a linear system of coupled equations. In the continuum regime they decouple into a set of

single-particle quantization conditions,

$$k_j = \frac{2\pi\lambda_j}{L-n}. \quad (7)$$

Here the length of the system is reduced by the exclusion volume taken by the finite size of the particles; see also Eq. (12) for a finite-range interaction below.

The adiabatic method we are using breaks down when a bound state is formed at a finite interaction strength while sweeping from $V = 0$ to $V = \infty$. Such states occur only when some of the quasimomenta of the solutions at $V = 0$ are $|k_j| > \pi/2$ (see Appendix and Ref. 20). The bound states can be observed, for instance, in the dynamics of a spin chain following a quench.²¹ In the continuum regime there is a wide range of model parameters where Eq. (7) is applicable: for momenta and energies in the spectral function smaller than $\pi/2$ and smaller than half bandwidth respectively.

The ground state is a band filled from the bottom up to the momentum $k_F = \pi(n-1)/L$ using the classification of Eq. (6). Here n is assumed odd for simplicity. Eigenstates involved in the form factors of the spectral function have a fixed number of particles $n+1$. All other eigenstates do not contribute to Eq. (2), as the number of particles is a conserved quantity.

In this paper, we are concerned with the location of the support of the spectral function (the lowest value of energy for which the spectral function is not zero) as opposed to its value, so we ignore the matrix elements in Eq. (2), assuming them to be nonzero for all f which satisfy the number constraint. Two δ functions in k and in ε map directly the total momenta and the eigenenergies of all many-body states $|f\rangle$ with $n+1$ particles into the shape of the spectral function. For a fixed value of k , the edge of the support is the smallest eigenenergy of all states $|f\rangle$, with $P_f = k$. Using the classification in Eq. (6), these states can be parametrized by a single variable ΔP [see the sketch in Fig. 2(b) and in the Appendix].

A. Low energies

At low energies the model of spinless fermions Eq. (1) is well approximated by the Tomonaga-Luttinger model with only two free parameters.¹ The first parameter is the slope of the linearized spectrum of excitations at k_F . For the states from Fig. 2(b) it is

$$v = \frac{L(E_2 - E_1)}{2\pi}, \quad (8)$$

where E_1 and E_2 are energies of the states with $\Delta P = 0$ and $\Delta P = 2\pi/L$, respectively. The second Luttinger parameter can be extracted as $K = v_F/v$,²² where $v_F = 2t\pi(n-1)/L$ is the Fermi velocity of the noninteracting system. The numerical evaluation of K as a function of the interaction strength V is presented in Fig. 1. For small V the function is linear, $K = 1 - 2n/L \times V/t + O(V^2/t^2)$. For large V it approaches a lower bound such that $K = K(\infty) + 2n/(L-n) \times t/V + O(t^2/V^2)$, where

$$K(\infty) = \left(1 - \frac{n}{L}\right)^2 \quad (9)$$

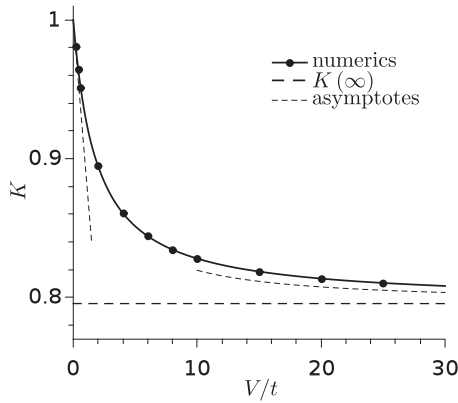


FIG. 1. The numerical evaluation of the Luttinger parameter K as a function of next-neighbor interaction strength V using Eqs. (3), (5), and (8), full ellipses; $L = 100$ and $n = 11$. We compare it with the bound on K at infinite interaction strength from Eq. (9), thick dashed line. Small and larger V asymptotes are $K = 1 - 2n/L \times V/t$ and $K = K(\infty) + 2n/(L - n) \times t/V$, thin dashed lines.

was computed using the values of quasimomenta for $V = \infty$ in Eq. (7).

The Luttinger parameter K measures the effects of interactions where for noninteracting particles $K = 1$. At $V = \infty$ the interaction potential is a hard-wall interaction with a finite interaction range, which still leaves some room for nonzero kinetic energy, thus limiting the maximum value of K .

B. High energies

The main aim of this paper is a calculation beyond low energies. In the nonlinear region the position of the edge of the spectral function is given by the momentum dependence of the states of Fig. 2(b), $\varepsilon_{\text{edge}}(k) = E_k - E_0$, where E_k corresponds to the states with $\Delta P = k_F + 2\pi/N - k$. For all values of V

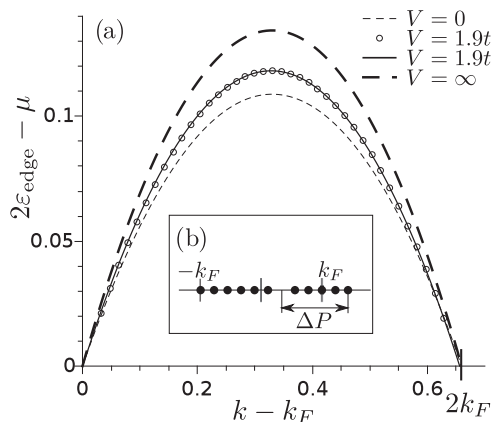


FIG. 2. (a) We show the main result of this paper, that the edge of the support of the spectral function satisfies Eq. (10). Numerical results at intermediate coupling ($V = 1.9t$) are shown as open circles and compared to the analytical result, Eq. (10), shown as a full line for $L = 400$ and $n = 39$. The asymptotes in the weak-coupling limit from Eq. (6) and the strong-coupling limit from Eq. (7) are shown as thin and thick dashed lines, respectively. (b) Sketch of the sets of quasimomenta, using classification Eq. (6), that correspond to the edge states; parameter ΔP corresponds to different momenta k .

we find it to be a parabolic function of momentum,

$$\varepsilon_{\text{edge}}(k) = \frac{mv_F^2}{K} - \frac{(k - 2mv_F)^2}{2mK}, \quad (10)$$

where $m = (2t)^{-1}$ is the bare single-electron mass and the Luttinger parameter K is determined by the slope at $k = k_F$. In the limiting cases $V = 0$ and $V = \infty$, it is calculated explicitly using the expressions for quasimomenta in Eqs. (6) and (7). The crossover for intermediate values of V is calculated using the numerical solution of the Bethe equations [Eq. (5)] and is perfectly fitted by the same parabolic formula [see Fig. 2(a)]. At $k = k_F$, Eq. (10) gives the chemical potential $\mu = mv_F^2/(2K)$, since the ground state for $n + 1$ particles is constructed by adding an extra particle to the ground state $|0\rangle$ at the lowest possible momentum above k_F , which is the state in Fig. 2(b) with $\Delta P = 0$.

The many-body states that mark the edge of the spectral function outside of the region $k_F < k < 3k_F$ are parametrized by a single variable similarly to Fig. 2(b) (see Appendix for details). In the upper half of the energy-momentum plane $\varepsilon > \mu$ the result in Eq. (10) is repeated along the momentum axis with the period $2k_F$. So $\varepsilon_{\text{edge}}(k)$ becomes $mv_F^2/K - (k - 2jmv_F)^2/(2mK) + \Delta\mu_j$ in regions $(2j - 1)k_F < k < (2j + 1)k_F$, with an additional shift $\Delta\mu_j$ for $|j| > 1$. The latter is given by the recurrence relation $\Delta\mu_{j+1} = \Delta\mu_j + 2|j|v_F/K$ with the initial value $\Delta\mu_1 = 0$. In the continuum regime of interest, $j \ll n$, $\Delta\mu_j$ is only a small finite size correction to μ . In the “hole region” $\varepsilon < \mu$, the position of the edge is obtained by reflection of $\varepsilon_{\text{edge}}(k)$ with respect to the line $\varepsilon = \mu$ (see Appendix).

A link between Luttinger liquids and the Fermi-edge singularity problem was very recently established as a tool to analyze interactions beyond the linear approximation in one dimension.¹² This has led to the development of a phenomenological theory of nonlinear Luttinger liquids where power-law singularities, $A(\varepsilon, k) \sim \theta[\varepsilon - \varepsilon_{\text{edge}}(k)]|\varepsilon - \varepsilon_{\text{edge}}(k)|^{-\alpha}$, were found above the edge of the support. Their exponents were related to the curvature of $\varepsilon_{\text{edge}}(k)$ for arbitrary momenta.¹² Substitution of Eq. (10) in the formula of Imambekov and Glazman from Ref. 13 yields

$$\alpha = 1 - \frac{K}{2} \left(1 - \frac{1}{K}\right)^2. \quad (11)$$

The Luttinger K of the model Eq. (1) (see Fig. 1) gives a divergent exponent smaller than 1 and larger than a limiting value calculated for $K(\infty)$ from Eq. (9). Thus the form factors in Eq. (2) are nonzero around the edge, thereby justifying our assumption about matrix elements in the spectral function.

IV. FINITE-RANGE INTERACTION

A further consequence of the non-linearity of the free particle dispersion is the bound on the Luttinger parameter K in Eq. (9). It has to be treated with care analogously to the point-splitting technique for field theoretical models,²³ in which a small interaction range must be introduced to couple a pair of fermions which cannot occupy the same point in space, and then the limit of zero range is taken. For the model on a lattice with next-neighbor coupling, the interaction

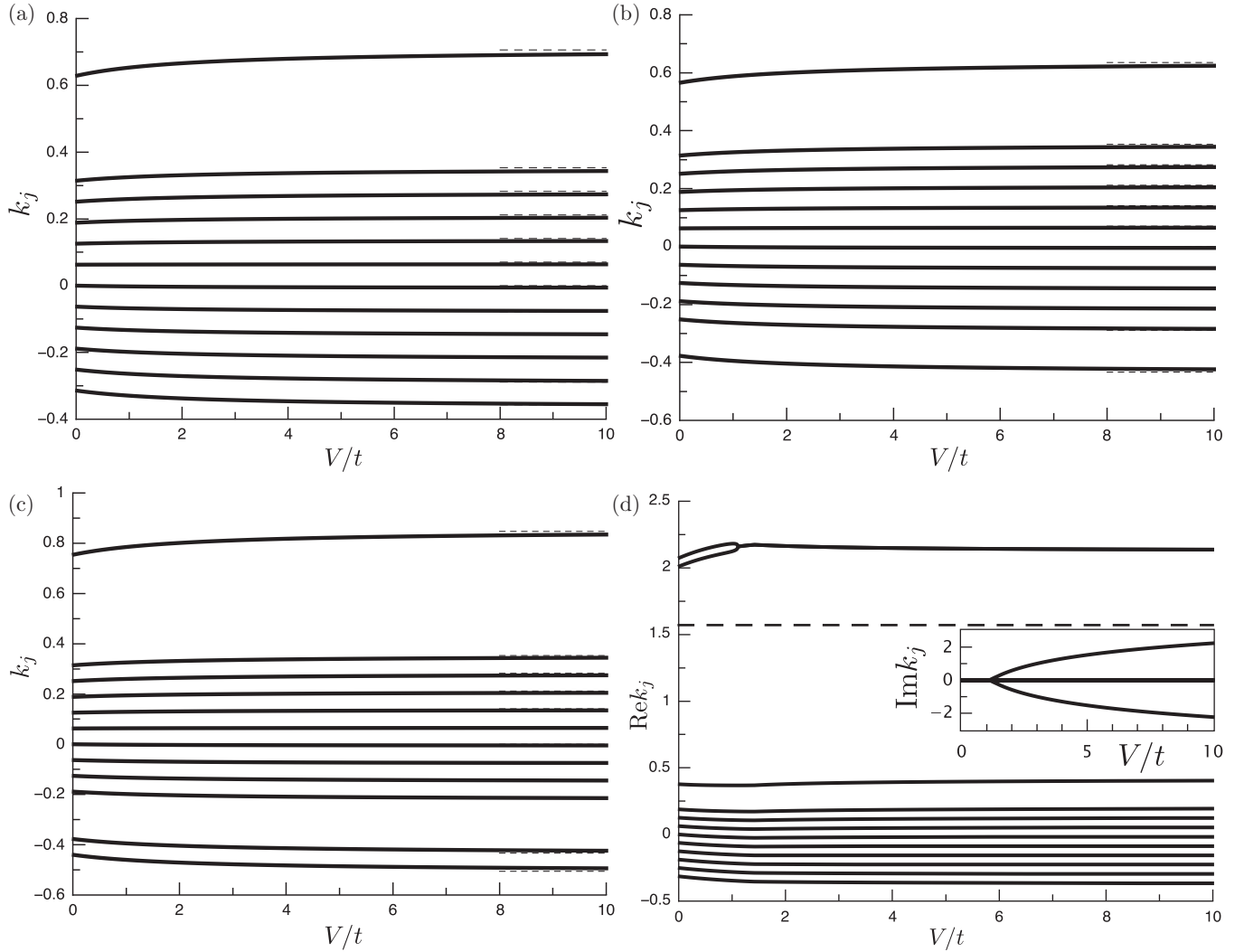


FIG. 3. The numerical solutions of Bethe equations, Eq. (5) of the main text, for k_j as a function of interaction strengths V for $n = 12$ particles and $L = 100$, full lines. The thin dashed lines at large V correspond to asymptotes from Eq. (7) of the main text. The states are classified according to Eq. (6) of the main text: (a) $\lambda_j = \{-5, -4, -3, -2, -1, 0, 1, 2, 3, 4, 10\}$; (b) $\lambda_j = \{-6, -4, -3, -2, -1, 0, 1, 2, 3, 4, 9\}$; (c) $\lambda_j = \{-7, -6, -3, -2, -1, 0, 1, 2, 3, 4, 12\}$; (d) $\lambda_j = \{-5, -4, -3, -2, -1, 0, 1, 2, 3, 6, 32, 33\}$. A bound state forms out of a pair of quasimomenta with $k_j > \pi/2$ above a finite value of V . The thick dashed line marks the value of $k = \pi/2$, and the inset is the imaginary parts of all quasimomenta k_j .

range vanishes in the continuum regime ($n \ll L$) compared to the average distance between particles; therefore $K(\infty) \rightarrow 1$, i.e., degenerate with its value for the noninteracting system $K(0) = 1$. However, the interaction range between fermions in physical systems is usually finite, e.g., the screening length for electrons in a metal or a semiconductor, making K not equal to 1. We, therefore, now consider a model with finite range.

We consider the limiting case of $V = \infty$ when the interaction range (screening length) spans a large number of lattice sites r . The Hamiltonian Eq. (1) with the potential $V_i = V\theta[i-1]\theta[r-]$, where $\theta[i]$ ($\theta[i] = 1$ for $i \geq 0$ and $\theta[i] = 0$ for $i < 0$) is a Heaviside step function and $V \rightarrow \infty$, can be diagonalized in the coordinate basis, $|\psi\rangle = \sum_{j_1 < j_2 - r \dots < j_n - r} a_{j_1 \dots j_n} c_{j_1}^\dagger \dots c_{j_n}^\dagger |\text{vac}\rangle$, by a superposition of plain waves, $a_{j_1 \dots j_n} = \sum_P e^{i \sum_{l=1}^n k_{P_l} j_l + i \sum_{l < m=1}^n \varphi_{P_l, P_m}}$, with $2\varphi_{jm} = (k_j - k_m)r + \pi$. Application of the periodic boundary

condition yields, similarly to Eq. (5),

$$k_j[L - r(n-1)] + r \sum_{m=1 \neq j}^n k_m = 2\pi\lambda_j, \quad (12)$$

which in the continuum regime gives a set of independent quantization conditions $k_j = 2\pi\lambda_j/(L - rn)$. Finally, by repeating the same calculation used to obtain Eq. (9) we find

$$K(\infty) = \left(1 - \frac{rn}{L}\right)^2, \quad (13)$$

where the term rn/L can be interpreted as a product of screening length and particle density.

A microscopic model of spinless fermions needs to have an interaction range of the order of the average distance between particles to reach the $K = 0$ value that corresponds

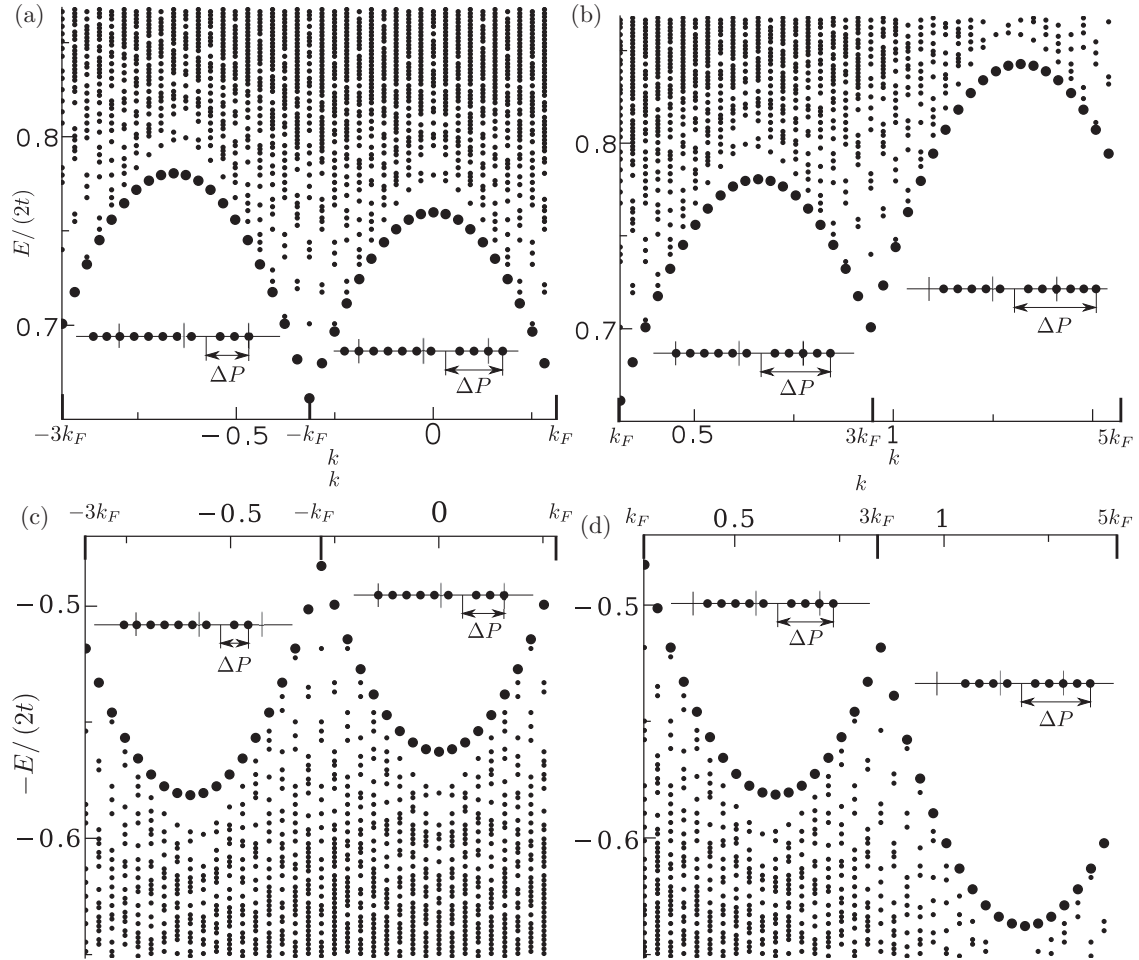


FIG. 4. Spectrum of the eigenstates, Eq. (3) of the main text, that are involved in the form factor in Eq. (2) of the main text for the ground state with $n = 19$ particles, $L = 200$, and $V \ll t$, dots. Large dots are the states at the edge. The insets are sketches of sets of quasimomenta that correspond to the edge states using the classification Eq. (6) of the main text. The positive half planes $E - E_0 > \mu$ are the states with an extra added particle: (a) momenta are from $-3k_F$ to k_F , the energies at the edge at $-3k_F$ and $-k_F$ correspond to chemical potentials μ_{-1} and μ_0 ; (b) momenta are from k_F to $5k_F$, the energies at the edge at k_F , $3k_F$, and $5k_F$ correspond to chemical potentials μ_1 , μ_2 , and μ_3 . The negative half planes $E_0 - E < \mu$ are the states with one particle removed: (c) momenta are from $-3k_F$ to k_F ; and (d) momenta are from k_F to $5k_F$.

to strong interaction effects in the Tomonaga-Luttinger model. Specifically, for $r = L/(2n)$, which allows some motion even when $V = \infty$, the bound is $K(\infty) = 1/4$. When r is increased further, $K(\infty)$ approaches zero.

V. CONCLUSIONS

In conclusion, we have considered the exact diagonalization of a model of spinless fermions on a lattice with next-neighbor interactions via the Bethe-Ansatz approach. By analyzing the spectral function in the continuum regime we have found that the edge of its support has a parabolic shape for arbitrary momenta and the prefactor is a function of the dimensionless Luttinger parameter K , which is defined in the low-energy domain. Additionally, we have extended our model with a finite range of interactions in order to access the strongly interacting regime (near $K = 0$) and have also found the parabolic shape for the support (for $V = \infty$), which is still characterized by K . This suggests that Luttinger parameters control physical properties at higher energies where nonlinearity cannot be ignored.

ACKNOWLEDGMENTS

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APPENDIX: NUMERICAL DATA

Here we present results of numerical calculations. Figure 1 shows some of the solutions to the Bethe-Ansatz equations, Eq. (5) of the main text, for different values of V . The states are parametrized using Eq. (6) of the main text. The states of Figs. 3(a)–3(c) have all $|k_j| < \pi/2$. The state of Fig. 3(d) contains a pair of $|k_j| > \pi/2$ that leads to formation of a bound state at a finite V . Figure 4 shows the extension of the edge beyond the region $k_F < k < 3k_F$ and $\varepsilon > \mu$. The eigenstates on the edge are marked by large dots and corresponding sets of quasimomenta are sketched in each region as insets.

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